

Table 2. Crystal data for the three new stacking variants

Layer type	Space group	Stacking order	Lattice constants (Å)†	
			Mg-Zn-Cu	Mg-Zn-Ag
8-layer	$P6_3/mmc$	$AB'AB'A'CA'C$	$a = 5.21$ $c = 34.2$	$a = 5.21$ $c = 34.4$
9-layer	$R\bar{3}m$	$AB'ABC'BCA'C$	$a = 5.19$ $c = 38.4$	$a = 5.21$ $c = 38.7$
10-layer	$P6_3/mmc$	$ABC'BCA'C'BC'B'$	$a = 5.17$ $c = 42.5$	$a = 5.22$ $c = 43.0$

† All the lattice constants are given for a hexagonal unit cell.

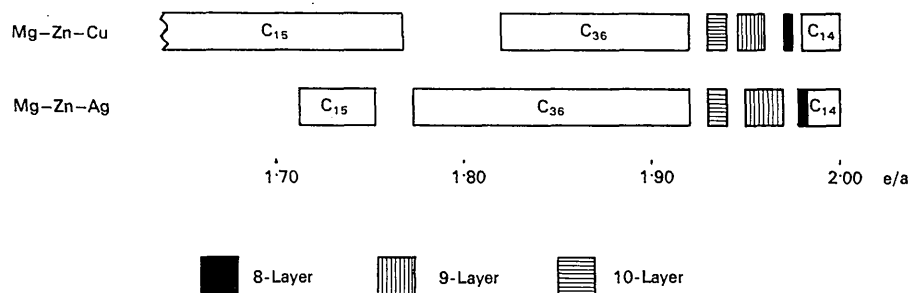


Fig. 2. Structural changes in the Mg-Zn-Cu and Mg-Zn-Ag alloys as a function of the electron-atom ratio.

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Remeasurements of the Structure of Potassium-2,2,5,5-tetramethyl-3-carboxypyrroline-1-oxyl

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The structure of the nitroxide free radical, $C_9H_{13}NO_3K \cdot \frac{1}{2}H_2O$ has been redetermined using data obtained for the full copper sphere with an automatic single-crystal diffractometer and $Mo K\alpha$ X-radiation. There are two independent molecules of the radical per asymmetric unit and after refinement to $R=0.07$ these were found to be identical and planar within experimental error. The irregularities observed in a previous investigation, particularly an abnormally short C-C bond which occurred in both crystallographically independent molecules in the asymmetric unit, did not recur and the expected molecular symmetry was observed.

Introduction

A crystal of the potassium salt of 2,2,5,5-tetramethyl-3-carboxypyrroline-1-oxyl was used previously (Kruger & Boeyens, 1968) to determine the geometry of a sterically protected nitroxide radical incorporated in a

five-membered ring. This system is important as a spin label (Hamilton & McConnell, 1968) and accurate structure parameters are desirable.

Because of insufficient data certain irregularities were observed, particularly for bonds lying parallel to [010]. The fact that one particular bond was similarly

Table 1. Fractional coordinates and anisotropic thermal parameters with their standard deviations

	x/a	y/b	z/c	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
				$T = \exp [-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$.					
K	0	0.6763 (3)	0.9537 (2)	0.0017 (1)	0.0102 (4)	0.0061 (2)	0	0	-0.0008 (3)
C(1)	0	0.0197 (15)	0.5981 (9)	0.0024 (3)	0.0121 (20)	0.0035 (7)	0	0	-0.0009 (10)
C(2)	0	0.1943 (14)	0.6711 (9)	0.0016 (2)	0.0126 (19)	0.0041 (7)	0	0	-0.0027 (10)
C(3)	0	0.3522 (16)	0.6123 (10)	0.0033 (3)	0.0128 (21)	0.0047 (8)	0	0	-0.0006 (11)
C(4)	0	0.3210 (17)	0.4840 (11)	0.0035 (4)	0.0171 (23)	0.0053 (10)	0	0	-0.0013 (13)
C(5)	0	0.1901 (16)	0.7967 (9)	0.0016 (2)	0.0151 (22)	0.0047 (7)	0	0	0.0006 (11)
C(6)	0.0622 (7)	0.3884 (17)	0.4259 (9)	0.0062 (5)	0.0312 (29)	0.0075 (8)	-0.0051 (10)	0.0041 (5)	-0.0023 (12)
C(8)	0.0611 (5)	0.8998 (13)	0.6119 (9)	0.0032 (3)	0.0199 (20)	0.0082 (8)	0.0034 (6)	-0.0006 (4)	-0.0026 (11)
O(1)	0	0.0163 (17)	0.3923 (9)	0.0052 (4)	0.0271 (28)	0.0064 (8)	0	0	-0.0049 (13)
O(2)	0	0.0311 (11)	0.8436 (7)	0.0024 (2)	0.0124 (14)	0.0048 (5)	0	0	0.0013 (8)
O(3)	0	0.3411 (11)	0.8501 (7)	0.0028 (2)	0.0136 (15)	0.0052 (6)	0	c	-0.0028 (8)
N	0	0.1086 (14)	0.4837 (9)	0.0031 (3)	0.0183 (20)	0.0051 (8)	0	0	-0.0023 (10)
K'	0.0927 (7)	0.1708 (2)	0	0.0018 (1)	0.0108 (2)	0.0064 (1)	-0.0001 (1)	-0.0003 (1)	0.0002 (2)
C(1')	0.2150 (4)	0.8478 (11)	0.2270 (7)	0.0019 (2)	0.0139 (15)	0.0063 (6)	0.0005 (4)	-0.0011 (3)	-0.0021 (9)
C(2')	0.1814 (3)	0.6668 (10)	0.1873 (6)	0.0016 (1)	0.0109 (12)	0.0044 (4)	-0.0008 (4)	-0.0007 (2)	-0.0006 (7)
C(3')	0.2067 (4)	0.5158 (11)	0.2318 (8)	0.0024 (2)	0.0109 (15)	0.0090 (8)	-0.0001 (5)	-0.0015 (4)	0.0004 (9)
C(4')	0.2644 (5)	0.5507 (12)	0.3073 (10)	0.0031 (3)	0.0132 (15)	0.0118 (10)	-0.0009 (6)	-0.0030 (5)	0.0024 (11)
C(5')	0.1258 (4)	0.6684 (10)	0.1083 (6)	0.0018 (2)	0.0129 (13)	0.0049 (5)	0.0002 (4)	-0.0008 (2)	-0.0004 (8)
C(6')	0.3277 (5)	0.4719 (16)	0.2(48 (13)	0.0027 (3)	c-0268 (26)	c-0174 (15)	0.0030 (8)	-0.0018 (6)	-0.0041 (17)
C(7')	0.2464 (7)	0.5067 (19)	0.4351 (10)	0.0059 (5)	0.0358 (30)	0.0076 (7)	-0.0053 (10)	-0.0028 (6)	0.0085 (15)
C(8')	0.2485 (5)	0.9358 (12)	0.1294 (8)	0.0030 (2)	0.0187 (19)	0.0076 (7)	-0.0031 (6)	-0.0010 (4)	0.0032 (10)
C(9')	0.1708 (5)	0.9743 (12)	0.3011 (10)	0.0026 (3)	0.0172 (18)	0.0105 (10)	0.0016 (6)	-0.0007 (4)	-0.0048 (11)
C(1')	0.3073 (3)	0.8629 (9)	0.3538 (7)	0.0031 (2)	0.0232 (15)	0.0114 (7)	-0.0009 (5)	-0.0035 (3)	0.0015 (9)
O(2')	0.1058 (3)	0.8254 (8)	0.0718 (6)	0.0031 (2)	0.0134 (11)	0.0097 (6)	-0.0007 (4)	-0.0028 (3)	0.0023 (8)
O(3')	0.1022 (3)	0.5119 (8)	0.0820 (6)	0.0029 (2)	0.0114 (10)	0.0097 (6)	-0.0002 (4)	-0.0020 (3)	-0.0031 (7)
N'	0.2665 (3)	0.7612 (9)	0.3002 (7)	0.0023 (2)	0.0167 (13)	0.0068 (6)	-0.0001 (4)	-0.0017 (3)	-0.0012 (7)
O(H ₂ O)	0	0.1068 (29)	0.1682 (10)	0.0038 (4)	0.0925 (17)	0.0068 (9)	0	0	-0.0010 (23)

Table 2 (cont.)

H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c	H _o F _o F _c
12 19 20	K _o 1, L _o 5	K _o 1, L _o 4	7 8 9	19 4 5	11 5 7	10 20 19	1 14 14	8 7 7	9 5 7	3 7 7	5 10 11				
13 16 17	0 23 21	1 5 5	9 6 6	10 7 7	12 4 4	12 21 21	11 9 8	11 9 8	12 10 10	2 11 7	6 10 9				
15 15 17	1 5 5	1 5 5	10 7 7	10 7 7	13 4 4	13 5 4	3 8 8	3 8 8	12 15 16	5 6 6	7 11 10				
16 8 8	2 4 5	3 9 7	11 17 17	22 4 4	14 5 5	14 10 11	4 4 5	16 8 7	14 5 6	9 10 11	8 5 5				
17 8 13	7 8 15	13 7 7	12 13 13	13 7 7	14 5 5	14 10 11	11 9 5	11 9 5	15 12 12	15 12 12	3 4 4				
18 8 8	4 10 9	7 9 9	13 7 7	0 37 37	10 11 9	16 9 9	6 8 9	6 8 9	18 4 2	18 4 2	10 8 7				
19 12 11	5 44 45	K _o 1, L _o 5	14 10 10	1 20 19	1 10 9	20 11 11	7 9 9	K _o 7, L _o 1	K _o 7, L _o 6	12 8 9	K _o 8, L _o 7				
20 6 6	1 4 2	1 4 2	15 11 13	2 7 7	2 7 7	22 10 10	11 11 11	7 9 9	0 21 21	7 9 9	12 8 9				
21 17 17	7 19 20	0 7 7	16 16 17	3 3 4	5 5 4	K _o 1, L _o 3	10 7 9	0 6 8	1 20 20	16 5 3	1 5 6				
22 7 7	8 5 7	1 4 2	17 9 9	4 10 9	4 10 9	0 11 11	11 9 5	5 13 14	2 4 3	3 7 5	2 5 2				
23 8 7	9 7 8	3 5 5	18 4 5	5 6 6	8 4 3	1 18 19	13 6 7	5 4 5	3 7 8	K _o 8, L _o 2	4 4 4				
25 5 1	10 3 3	4 6 5	19 6 5	6 16 16	9 6 6	2 4 3	14 6 6	6 18 18	4 8 8	0 14 16	4 7 7				
K _o 1, L _o 1	11 4 4	2 0 4	20 4 5	7 3 5	10 4 6	5 11 10	15 12 5	5 15 15	5 15 15	1 12 12	5 9 10				
0 52 51	12 3 3	0 3 4	21 4 4	8 14 14	11 6 5	4 13 14	17 5 6	8 13 13	6 9 11	2 6 6	12 11 11				
1 13 14	13 11 11	1 11 11	22 7 7	9 9 8	12 5 5	5 38 38	18 4 3	10 5 5	7 11 11	3 6 6	7 8 7				
2 19 20	15 13 14	2 7 9	23 5 5	10 13 12	10 13 12	6 10 5	19 9 7	12 5 5	9 15 16	4 4 6	K _o 8, L _o 9				
3 10 10	16 7 6	3 9 9	K _o 5, L _o 6	11 13 12	0 13 14	7 6 5	20 9 8	13 7 9	10 5 2	5 9 9	0 6 5				
4 19 20	17 15 16	3 9 9	0 20 10	12 11 11	6 9 8	8 6 5	0 18 19	14 6 6	11 12 13	6 6 5	1 4 3				
5 21 21	19 4 4	5 24 24	1 21 20	13 6 6	2 4 4	9 17 16	2 6 6	16 16 16	13 9 9	9 7 5	2 3 2				
6 34 32	K _o 1, L _o 6	6 22 20	2 3 1	14 6 8	5 5 4	10 4 4	3 6 6	18 11 10	14 5 5	9 10 11	4 8 8				
7 25 15	0 18 19	7 19 15	3 4 5	15 4 4	4 7 6	11 16 16	4 9 9	K _o 7, L _o 2	15 5 6	10 11 12	5 7 6				
8 25 15	1 4 3	9 11 11	4 32 35	16 7 7	8 5 3	12 5 4	5 4 4	0 13 11	17 8 7	11 6 6	6 5 6				
9 15 14	2 13 12	10 5 3	5 33 33	17 4 3	9 5 6	13 14 13	6 16 17	1 4 3	K _o 7, L _o 7	12 4 6	7 4 2				
10 28 30	3 4 3	11 27 27	6 31 32	18 4 5	10 5 5	14 6 5	7 4 4	2 5 5	0 22 21	13 6 8	K _o 9, L _o 10				
11 14 14	4 14 14	12 9 10	7 11 10	22 6 7	0 5 5	15 12 13	8 10 10	3 22 21	1 5 7	14 5 4	3 6 8				
12 23 22	5 13 14	15 9 10	8 15 16	K _o 5, L _o 1	0 5 5	17 7 7	9 6 6	5 15 16	2 10 11	15 1 5	4 3 5 17				
14 10 11	6 13 12	16 13 13	9 8 10	10 23 20	1 7 7	18 5 5	10 13 13	7 22 21	4 7 9	16 7 9	5 4 5				
15 7 8	7 6 7	17 19 19	10 9 10	1 16 15	3 4 4	19 6 6	11 4 2	9 8 9	6 7 7	0 10 11	6 19 21				
16 15 15	8 12 12	18 6 6	11 24 23	2 6 9	4 5 5	20 6 6	14 6 5	10 6 7	8 7 7	K _o 9, L _o 1	7 7 7				
17 14 4	10 13 12	22 4 5	12 13 12	4 8 6	5 5 5	21 10 10	16 11 12	11 6 7	9 4 4	1 9 11	7 7 7				
18 10 11	11 5 4	25 4 3	13 3 3	6 8 8	K _o 5, L _o 10	K _o 5, L _o 10	18 9 9	12 4 3	10 17 18	2 7 8	10 6 6				
19 5 5	12 7 7	1 0 4 4	14 10 10	7 9 9	0 19 19	7 9 9	0 19 19	7 9 9	12 4 3	10 6 6	K _o 9, L _o 10				
20 11 11	13 3 1	0 4 4	15 12 12	8 5 5	1 22 22	1 6 6	0 3 2	14 4 3	12 18 2	4 7 7	10 10 10				
21 3 3	15 6 4	1 3 2	16 12 11	11 11 11	2 26 24	2 6 6	0 10 10	15 14 14	14 6 7	8 5 5	1 9 9				
22 13 15	4 4 4	2 7 7	17 10 10	10 10 10	3 15 16	3 15 16	2 8 8	16 6 7	16 6 7	6 7 6	5 4 5				
24 5 5	16 8 7	3 8 7	18 8 8	9 11 14	4 13 10	4 24 25	3 10 11	17 13 13	16 8 7	7 6 6	4 7 7				
25 6 5	5 6 6	4 26 25	19 4 4	12 10 10	5 5 5	5 5 5	5 5 5	18 9 9	8 7 7	4 4 4	5 15 17				
K _o 1, L _o 10	K _o 1, L _o 10	5 25 26	20 4 3	13 6 6	6 7 7	6 17 17	5 18 19	19 5 6	K _o 8, L _o 6	9 8 10	5 15 17				
0 25 25	1 11 11	6 33 32	21 5 6	14 7 6	8 18 19	7 12 12	6 5 6	20 6 7	1 18 18	10 7 7	7 12 11				
1 32 31	2 5 5	7 19 19	22 5 5	15 6 6	9 13 13	8 10 11	7 15 16	K _o 7, L _o 1	4 4 3	11 9 10	9 5 7				
2 28 30	3 14 14	8 21 21	23 8 7	16 8 7	10 52 53	10 9 10	8 5 5	0 18 16	5 5 7	12 9 9	11 8 8				
3 26 25	4 10 10	9 13 15	0 15 12	K _o 5, L _o 5	18 5 5	11 10 9	9 4 4	1 6 5	7 4 3	3 7 7	11 8 8				
4 8 7	5 19 19	10 17 15	0 17 12	20 4 3	12 23 23	13 4 5	10 4 3	3 2 6	6 8 1	16 6 7	10 10 10				
5 23 23	6 5 7	12 10 10	1 25 24	K _o 5, L _o 9	13 10 10	14 7 7	11 6 6	3 6 6	9 8 8	K _o 8, L _o 1	4 4 1				
6 4 4	7 11 12	13 11 12	2 25 16	14 15 15	15 15 15	16 11 7	12 7 6	4 7 6	10 15 7	11 6 7	3 4 15				
7 25 25	8 4 5	15 13 14	3 13 15	1 14 13	18 8 6	17 7 6	17 13 12	5 9 9	11 15 15	1 6 7	4 14 15				
8 6 5	11 4 3	16 18 18	4 33 34	2 11 10	19 8 8	19 4 2	0 10 10	6 25 27	15 7 6	2 12 12	6 15 17				
9 25 25	14 3 5	17 11 11	5 25 26	3 8 8	20 13 13	20 5 2	14 8 8	18 5 4	16 7 6	3 8 7	5 7 9				
10 20 21	15 9 10	18 12 12	6 23 22	6 7 8	21 5 4	21 5 4	2 16 16	8 8 9	0 11 11	5 9 10	8 6 5				
11 20 22	16 4 4	19 4 4	7 14 14	8 4 4	22 14 14	22 5 5	3 10 10	10 8 8	2 9 9	10 10 10	10 8 8				
12 10 10	18 4 4	20 7 7	8 17 17	9 7 7	23 6 6	23 6 6	2 5 5	6 8 9	3 6 8	11 10 11	10 8 8				
13 11 11	19 3 3	9 20 20	9 8 7	9 7 7	K _o 6, L _o 1	0 17 18	7 5 4	12 6 5	4 6 6	10 11 11	1 10 11				
14 10 10	K _o 1, L _o 11	10 22 22	10 9 9	0 6 7	10 12 6	11 12 6	14 12 12	6 4 4	14 12 12	12 9 9	K _o 9, L _o 1				
15 20 21	0 10 9	25 6 4	11 15 15	11 12 12	1 43 45	2 5 5	10 6 7	15 4 4	8 5 2	13 5 3	2 9 8				
16 6 6	1 4 3	K _o 5, L _o 2	12 4 4	5 12 14	2 15 17	3 9 10	12 7 6	16 10 10	10 11 13	15 5 5	4 4 4				
17 13 10	2 5 4	0 9 9	13 10 10	3 8 8	3 26 26	4 6 7	16 11 11	12 10 10	12 10 10	1 9 9	10 10 10				
18 6 4	3 4 6	1 15 12	14 9 9	14 5 3	4 6 7	6 10 8	15 5 3	K _o 7, L _o 4	0 12 14	10 7 7	7 7 8				
19 9 9	4 14 15	2 11 11	15 6 5	16 4 4	5 24 25	5 14 15	0 9 8	1 10 10	1 9 8	5 8 5	4 4 4				
20 7 8	5 4 3	3 23 25	16 6 6	17 14 9	6 11 4	9 6 7	7 7 6	10 8 8	3 7 5	2 4 9	8 5 4				
21 9 9	6 9 10	4 33 33	17 9 9	19 4 2	7 22 22	10 6 5	3 10 9	2 7 7	5 5 4	4 6 6	11 11 10				
23 8 7	5 8 22	K _o 5, L _o 10	18 6 7	20 7 7	8 10 11	11 20 21	5 10 11	11 20 21	6 4 1	5 12 12	K _o 9, L _o 1				
K _o 1, L _o 7	10 6 6	6 27 26	19 4 4	0 11 11	9 23 24	12 5 5	5 18 18	2 4 6	6 9 9	6 7 7	7 7 7				
0 29 29	11 4 7	7 29 31	20 5 4	1 11 10	11 10 10	13 8 9	6 5 5	5 33 33	10 5 3	7 6 6	1 5 6				
1 9 14	6 7 7	8 25 25	21 8 2	2 7 7	12 12 22	17 9 9	7 8 8	6 8 8	11 9 6	10 8 6	2 8 7				
2 13 13	10 7 5	9 15 16	22 5 6	3 8 8	8 8 8	12 14 15	21 6 7	8 5 3	7 12 13	10 8 10	4 7 8				
3 10 10	18 4 5	10 8 8	23 6 6	4 5 5	13 8 8	K _o 1, L _o 6	5 7 6	0 6 8	6 8 8	5 5 4	4 4 4				
4 32 32	K _o 1, L _o 12	11 5 3	0 19 20	8 4 4	15 11 9	1 3 5	11 6 6	10 4 4	6 7 5	12 10 10	5 5 3				
5 13 12	0 7 6	12 9 8	0 19 20	8 4 4	15 11 9	1 3 5	11 6 6	10 4 4	6 7 5	12 10 10	5 5 3				
6 13 16	10 6 5	13 12 12	12 8 8	9 6 5	16 10 6	2 17 19	13 7 6	8 8 8	11 9 8	10 8 8	6 5 3				
7 17 16	3 8 7	14 11 11	2 16 16	10 11 10	17 4 3	3 7 7	7 7 7	K _o 1, L _o 12	12 6 5	0 16 14	0 12 13				
8 32 32	4 4 3	15 17 17	3 6 5	11 13 13	18 6 6	4 9 8	0 7 8	13 11 10	1 15 4	1 15 4	10 10 10				
9 8 7	5 13 13	16 17 17	4 9 8	12 11 9	19 6 6	5 6 6	1 5 5	14 4 2	2 12 12	7 4 3	10 10 10				
10 13 12	6 6 5	17 11 12	5 15 15	13 7 5	21 12 12	6 12 13	3 4 4	15 15 16	4 4 2	3 7 6	4 4 4				
11 4 5	7 9 8	18 11 10	6 17 17	14 2 2	22 6 6	7 5 4	4 8 8	16 5 5	5 4 8	8 8 8	5 4 4				
12 5 9	13 4 4	19 6 6	4 3 17	6 6 6	23 7 7	8 15 16	6 13 13	17 12 12	6 4 1	5 7 8	5 4 4				
14 15 15	14 4 3	20 6 5	8 10 11	0 5 5	K _o 5, L _o 11	K _o 5, L _o 11	10 8 8	18 5 4	8 13 11	6 7 7	0 9 9				
15 4 4	15 7 7	21 6 7	9 16 16	1 10 9	0 30 30	11 3 3	9 10 9	K _o 7, L _o 1	13 11 11	10 11 11	1 6 7				
16 20 20	K _o 1, L _o 13	24 5 3	10 10 9	1 6 6	2 27 25	12 13 14	K _o 1, L _o 1	0 22 23	11 13 14	8 8 5	5 5 5				
17 6 6	0 7 8	K _o 5, L _o 3	11 14 14	2 4 4	3 7 9	13 3 1	1 6 6	3 6 5	12 13 13	10 7 8	3 6 4				
18 10 10	1 4 2	0 22 23	12 8 8	3 4 3	4 22 21	14 4 5	2 18 18	4 10 10	2 16 16	11 8 7	4 9 8				
19 3 3	1 4 2	1 20 21	13 6 4	4 4 4	5 9 9	15 3 3									

data. The length of the nitroxide N–O bond is now also closer to the value of 1.26 Å found by Lajzėrowicz-Bonneteau (1968) in a similar compound.

Table 4. Observed molecular bond lengths and angles

Bond	Molecule	
	Mirror plane	General position
C(1)–C(2)	1.504 ± 0.014 Å	1.529 ± 0.009 Å
C(2)–C(3)	1.315 ± 0.015	1.299 ± 0.010
C(3)–C(4)	1.533 ± 0.016	1.510 ± 0.012
C(4)–N	1.501 ± 0.015	1.490 ± 0.010
N–C(1)	1.492 ± 0.015	1.502 ± 0.010
N–O(1)	1.263 ± 0.013	1.277 ± 0.008
C(2)–C(5)	1.486 ± 0.014	1.481 ± 0.009
C(5)–O(2)	1.253 ± 0.013	1.260 ± 0.009
C(5)–O(3)	1.239 ± 0.013	1.248 ± 0.009
O(3)–K	2.666 ± 0.008	2.605 ± 0.006
C(1)–C(8)	1.529 ± 0.011	1.558 ± 0.012
C(1)–C(9)		1.549 ± 0.012
C(4)–C(6)	1.534 ± 0.012	1.509 ± 0.015
C(4)–C(7)		1.587 ± 0.015
H ₂ O–N	2.726 ± 0.016	
H ₂ O–K		2.798 ± 0.009
Angle		
C(1)–C(2)–C(3)	113.1 ± 0.9°	112.3 ± 0.6°
C(2)–C(3)–C(4)	113.6 ± 1.0	115.1 ± 0.7
C(3)–C(4)–N	98.4 ± 1.0	98.8 ± 0.7
C(4)–N–C(1)	114.8 ± 0.9	114.7 ± 0.7
N–C(1)–C(2)	100.1 ± 0.9	99.1 ± 0.6
C(1)–N–O(1)	124.0 ± 0.9	121.7 ± 0.6
C(4)–N–O(1)	121.2 ± 1.1	123.6 ± 0.7
C(1)–C(2)–C(5)	123.8 ± 1.0	122.7 ± 0.6
C(2)–C(5)–O(2)	117.4 ± 1.0	118.5 ± 0.6
C(2)–C(5)–O(3)	119.5 ± 1.0	117.0 ± 0.7
C(5)–O(3)–K	176.7 ± 0.8	160.4 ± 0.6
C(6)–C(4)–C(7)	114.0 ± 1.3	116.6 ± 1.0
N–C(4)–C(6)	108.0 ± 0.7	108.9 ± 0.9
N–C(4)–C(7)		104.8 ± 0.9
C(8)–C(1)–C(9)	111.3 ± 1.0	113.0 ± 0.7
N–C(1)–C(8)	109.3 ± 0.6	108.6 ± 0.7
N–C(1)–C(9)		109.1 ± 0.7
C(2)–C(1)–C(8)	113.1 ± 0.6	113.3 ± 0.7
C(2)–C(1)–C(9)		112.8 ± 0.6
C(3)–C(4)–C(6)	113.5 ± 0.7	115.3 ± 1.0
C(3)–C(4)–C(7)		110.3 ± 0.9

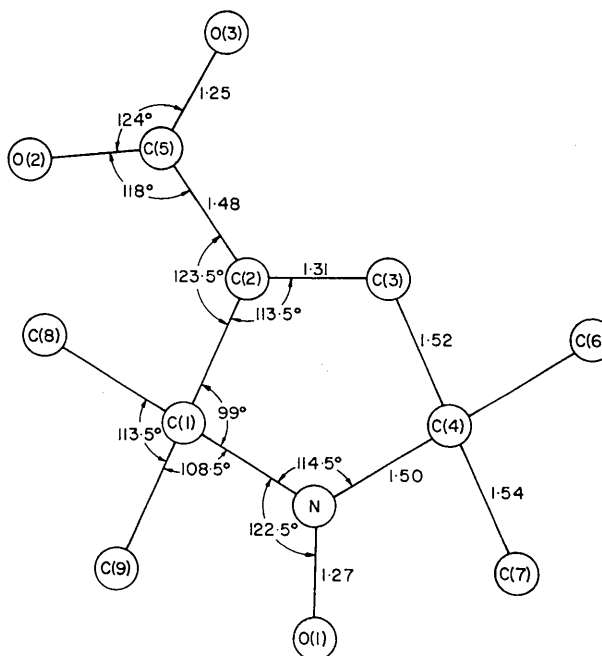


Fig. 1. Geometry of the organic anion averaged over chemically equivalent bonds and angles and assuming *mm* symmetry for the nitroxide ring.

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